

ABSTRACT

Method for developing a quantitative structure activity relationship that includes obtaining a training set of chemical compounds with molecular descriptors consisting of a number of multidimensional vectors with an activity class for each of the vectors; partitioning the multidimensional vectors into groups having interdependence; transforming the descriptors such that the interdependence of the groups is lessened; estimating a probability distribution of the descriptors by assuming that a probability distribution of a product of each of the groups is approximately equal to the probability distribution of the molecular descriptors; performing the partitioning, transforming and estimating steps for each of the activity classes; and, developing a probability distribution for the activity classes.